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Multiscale Problems in Materials Science: A Mathematical Approach to the Role of Uncertainty

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14. ABSTRACT The bottom line of this work is to develop affordable numerical methods in the context of stochastic homogenization. Many partial differential equations of materials science indeed involve highly oscillatory coefficients and small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic random problems (and the associated stochastic homogenization theory) are one instance for modelling uncertainty in continuous media. The theoretical aspects of these problems are now well-understood, at least for a large variety of situations. On the other hand, the numerical aspects have received less attention from the mathematics community. Standard methods available in the literature often lead to very, and sometimes prohibitively, costly computations. In this report, we first review an approach popular in particular in the computational mechanics community, which is to try and obtain bounds on the homogenized matrix, rather than computing it. Only computations of moderate difficulty are then required. However, we will show that, not unexpectedly, this method has strong limitations. We will next introduce a class of materials of significant practical relevance, that of random materials where the amount of randomness is small. They can be considered as stochastic perturbations of deterministic materials, in a sense made precise below. We will adapt to such a case the well-known Multiscale Finite Element Method (MsFEM), and design a method which is much more affordable than, and as accurate as, the original method.					
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Multiscale problems in materials science:
a mathematical approach to the role of uncertainty

Report 2010 to the European Office of
Aerospace Research and Development (EOARD)

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Summary

We report here on the work performed during the first year (october 2009 - october 2010) of the contract FA 8655-10-C-4002 on *Multiscale problems in materials science: a mathematical approach to the role of uncertainty*.

The bottom line of our work is to develop *affordable numerical methods* in the context of *stochastic homogenization*. Many partial differential equations of materials science indeed involve highly oscillatory coefficients and small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic random problems (and the associated stochastic homogenization theory) are one instance for modelling uncertainty in continuous media. The theoretical aspects of these problems are now well-understood, at least for a large variety of situations.

On the other hand, the numerical aspects have received less attention from the mathematics community. Standard methods available in the literature often lead to very, and sometimes prohibitively, costly computations.

In this report, we first review an approach popular in particular in the computational mechanics community, which is to try and obtain *bounds* on the homogenized matrix, rather than computing it. Only computations of moderate difficulty are then required. However, we will show that, not unexpectedly, this method has strong limitations.

We will next introduce a class of materials of significant practical relevance, that of random materials where the amount of randomness is *small*. They can be considered as *stochastic perturbations of deterministic materials*, in a sense made precise below. We will adapt to such a case the well-known Multiscale Finite Element Method (MsFEM), and design a method which is much more affordable than, and as accurate as, the original method.

The works described below have been performed by Claude Le Bris (PI), Frédéric Legoll (Co-PI), and Florian Thomines (first year Ph.D. student).

1 Introduction

Many partial differential equations of materials science involve highly oscillatory coefficients and small length-scales. Homogenization theory is concerned with the derivation of averaged equations from the original oscillatory equations, and their treatment by adequate numerical approaches. Stationary ergodic random problems are one of the most famous instances of mathematical uncertainty of continuous media. However, the elaborate tools and techniques of (i) mathematical probability, stochastic analysis, and (ii) numerical analysis and large-scale computing have not yet permitted practical computations. These are most often accomplished otherwise by the engineering community, using more traditional approaches. Despite definite achievements by leading experts, numerical analysis of stochastic, and more generally speaking non periodic, homogenization problems remains in its infancy.

The purpose of this report is to present the recent progress we have made during last year on this topic, with the aim *to make numerical random homogenization more practical*. Because we cannot embrace all difficulties at once, the case under consideration here is a *simple, linear, scalar second order elliptic partial differential equation in divergence form*, for which a sound

theoretical groundwork exists. We focus here on different practical computational approaches.

This report begins, in Section 2, with a brief introduction to stochastic homogenization. There is of course no novelty in such an introduction, the only purpose of which is the consistency of this report and the convenience of the reader not familiar with the theory. We will recall there why stochastic homogenization often leads to extremely expensive computations.

In Section 3, we describe a classical approach from the applied communities, which is to try and obtain *bounds* on the homogenized matrix, rather than computing it. The computational gain is evident. We will report on some numerical experiments. Such experiments are likely to not be new. But they at least show, quantitatively and qualitatively, the strong limitations of such an approach.

As pointed out above, random homogenization for general stochastic materials is very costly. Yet, it turns out that it is possible to identify classes of materials of significant practical relevance, where stochastic homogenization theory and practice can be reduced to more affordable, less computationally demanding problems. These materials are neither periodic (because such an oversimplifying assumption is rarely met in practice), nor fully stochastic. They can be considered as an intermediate case, that of *stochastic perturbations of deterministic (possibly periodic) materials*. The case when the tensor describing the properties of the material is the sum of a periodic term and a small random term is an instance of such an approach. In Section 4, we show that we can adapt to that particular setting the well-known Multiscale Finite Element Method (MsFEM), which is designed to directly address the highly oscillating elliptic problem, rather than studying the limit problem when the typical small lengthscale goes to 0. This method has been initially proposed for deterministic problems [24, 21, 22, 14], and has been recently adapted to the stochastic setting [18]. It then leads to extremely intensive computations. We show in the sequel that, if the problem is only weakly stochastic, then it is possible to design a method as accurate as the original MsFEM, with a much smaller computational cost. As we explain below, this method is accurate provided the stochastic perturbation is indeed small.

We collect in Section 5 some conclusions about the work performed so far, and future directions for the next two years of contract.

2 Basics of stochastic homogenization

[Detailed presentation can be read in [1].]

Stochastic homogenization is best understood in the light of the easiest context of homogenization: *periodic* homogenization. This is the reason why we begin with Section 2.1 laying some groundwork in the periodic context, before turning to stochastic homogenization *per se* in Section 2.2.

We refer to, *e.g.*, the monographs [15, 19, 25] for more details on homogenization theory, and to the review article [1] that we wrote, addressing some computational challenges in numerical stochastic homogenization. A super elementary introduction is contained in [13].

In this section, we present classical results of the literature. The reader familiar with stochastic homogenization can proceed directly to our contributions, detailed in Sections 3 and 4.

2.1 Periodic homogenization

For consistency, we recall here some basic ingredients of elliptic homogenization theory in the periodic setting. We consider, in a regular bounded domain \mathcal{D} in \mathbb{R}^d , the problem

$$\begin{cases} -\operatorname{div} \left[A_{per} \left(\frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right] = f & \text{in } \mathcal{D}, \\ u^\varepsilon = 0 & \text{on } \partial\mathcal{D}, \end{cases} \quad (1)$$

where the matrix A_{per} is symmetric definite positive and \mathbb{Z}^d -periodic. We manipulate for simplicity *symmetric* matrices, but the discussion carries over to non symmetric matrices up to slight modifications.

The microscopic problem associated to (1), called the *corrector problem* in the terminology of homogenization theory, reads, for p fixed in \mathbb{R}^d ,

$$\begin{cases} -\operatorname{div} (A_{per}(y) (p + \nabla w_p)) = 0 & \text{in } \mathbb{R}^d, \\ w_p \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases} \quad (2)$$

It has a unique solution up to the addition of a constant. Then, the *homogenized* coefficients read

$$[A^\star]_{ij} = \int_Q (e_i + \nabla w_{e_i}(y))^T A_{per}(y) e_j dy, \quad (3)$$

where Q is the unit cube, and where w_{e_i} denotes the solution to (2) for $p = e_i$, with e_i the canonical vectors of \mathbb{R}^d . The main result of periodic homogenization theory is that, as ε goes to zero, the solution u^ε to (1) converges to u^\star solution to

$$\begin{cases} -\operatorname{div}[A^\star \nabla u^\star] = f & \text{in } \mathcal{D}, \\ u^\star = 0 & \text{on } \partial\mathcal{D}. \end{cases} \quad (4)$$

Several other convergences on various products involving $A_{per}\left(\frac{x}{\varepsilon}\right)$ and u^ε also hold. All this is well documented.

The practical interest of the approach is evident. No small scale ε is present in the homogenized problem (4). At the price of only computing d periodic problems (2) (as many problems as dimensions in the ambient space) the solution to problem (1) can be efficiently approached for ε small. A direct attack of problem (1) would require taking a meshsize smaller than ε . The difficulty has been circumvented. Of course, many improvements and alternatives exist in the literature.

2.2 Stochastic homogenization

The mathematical setting of stochastic homogenization is more involved than that of the periodic case.

We put ourselves in the usual probability theoretic setting for *stationary ergodic homogenization*, with the exception that our notion of stationarity is *discrete*. It intuitively means the following. Pick two points x and $y \neq x$ at the microscale in the material and assume $y = x + k$ with $k \in \mathbb{Z}^d$. The particular local environment seen from x (that is, the microstructure present at x) is generically different from what is seen from y (that is, the microstructure present at y). However, the *average* local environment in x is assumed to be identical to that in y (considering the various realizations of the random material). In mathematical terms, the *law* of microstructures is the same. This is *stationarity*. On the other hand, *ergodicity* means that considering all the points in the material amounts to fixing a point x in this material and considering all the possible microstructures present there.

2.2.1 Main result

With the same setting as that described for periodic homogenization, we may now briefly describe the main result of stochastic homogenization. The

solution u^ε to the boundary value problem

$$\begin{cases} -\operatorname{div} \left(A \left(\frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right) = f & \text{in } \mathcal{D}, \\ u^\varepsilon = 0 & \text{on } \partial \mathcal{D}, \end{cases} \quad (5)$$

converges, when $\varepsilon \rightarrow 0$, to the solution u^* of (4) where the homogenized matrix is now

$$[A^*]_{ij} = \mathbb{E} \left(\int_Q (e_i + \nabla w_{e_i}(y, \cdot))^T A(y, \cdot) e_j dy \right). \quad (6)$$

The corrector problem now reads

$$\begin{cases} -\operatorname{div} [A(y, \omega) (p + \nabla w_p(y, \omega))] = 0 & \text{on } \mathbb{R}^d, \\ \nabla w_p \text{ is stationary, } \mathbb{E} \left(\int_Q \nabla w_p(y, \cdot) dy \right) = 0. \end{cases} \quad (7)$$

A striking difference between the stochastic setting and the periodic setting can be observed comparing (2) and (7). In the periodic setting, the corrector problem is posed on a *bounded* domain, namely the periodic cell Q . In sharp contrast, the corrector problem (7) of the random setting is posed on the *whole space* \mathbb{R}^d , and cannot be reduced to a problem posed on a bounded domain. The reason is, condition $\mathbb{E} \left(\int_Q \nabla w_p(y, \cdot) dy \right) = 0$ in (7) is a *global* condition. It indeed equivalently reads, because of the ergodic theorem, $\lim_{R \rightarrow +\infty} \frac{1}{|B_R|} \int_{B_R} \nabla w_p(y, \cdot) dy = 0$ for any sequence of balls B_R of radii R .

The fact that the random corrector problem is posed on the entire space has far reaching consequences for numerical practice. Actually, this is probably the main source of all the *practical difficulties* of stochastic homogenization.

2.2.2 The direct numerical approach

Practical approximations of the homogenized problem in random homogenization are not easily obtained, owing to the fact that the corrector problem (7) is set on the entire space. In practice, truncations have to be considered, and the actual homogenized coefficients are only obtained in the asymptotic regime.

Let us now be more explicit. In practice, the matrix A^\star is approximated by the matrix

$$[A_N^\star]_{ij}(\omega) = \frac{1}{|Q_N|} \int_{Q_N} (e_i + \nabla w_{e_i}^N(y, \omega))^T A(y, \omega) (e_j + \nabla w_{e_j}^N(y, \omega)) dy, \quad (8)$$

which is in turn obtained by solving the corrector problem on a *truncated* domain, say the cube $Q_N = (-N, N)^d \subset \mathbb{R}^d$:

$$\begin{cases} -\operatorname{div} (A(\cdot, \omega) (p + \nabla w_p^N(\cdot, \omega))) = 0 & \text{on } \mathbb{R}^d, \\ w_p^N(\cdot, \omega) \text{ is } Q_N\text{-periodic.} \end{cases} \quad (9)$$

Although A^\star itself is a deterministic object, its practical approximation A_N^\star is random. It is only in the limit of infinitely large domains Q_N that the deterministic value is attained (the convergence $\lim_{N \rightarrow \infty} A_N^\star(\omega) = A^\star$ has been shown in [16, Theorem 1]).

At fixed N , the approximate homogenized matrix A_N^\star is random: a set of M independent realizations of the random coefficient A are therefore considered. The corresponding truncated problems (9) are solved, and an empirical mean of the truncated coefficients (8) is inferred. This empirical mean only agrees with the theoretical mean value of the truncated coefficient within a margin of error which is given by the central limit theorem (in terms of M). For a sufficiently large truncation size N , this truncated value is admittedly the exact value of the coefficient. The overall computation described above is thus very expensive, because each realization requires a new solution to the problem (9) of presumably large a size since N is taken large.

3 Bounds for homogenization

[Work expanded in [1].]

Given the above computational workload, practitioners, especially scientists from the applied communities (computational mechanics, ...), sometimes choose to avoid computing actual homogenized equations and concentrate on *bounds* on the homogenized matrices A^\star . In [1], we have carefully studied this approach, which has some (strong, as will be seen below) limitations.

We consider here the specific case of composite materials consisting of only two phases. We denote by A and B the associated matrix coefficients, modelling the properties of the phases. We also fix the average volume fraction θ of the phase A . For simplicity, we assume here that θ is uniform over the whole material. The problem is to find all possible homogenized materials, that is, mathematically, matrices A^* , that can be attained homogenizing such phases A and B with the volume fraction θ .

In this specific case, some bounds on the homogenized coefficients may be established. Here, we present one example of such bounds (actually the most famous one). The case we consider is a scalar equation of the type (1) with a matrix coefficient $A^\varepsilon(x)$ that needs not be periodic, nor stationary ergodic, and that reads

$$A^\varepsilon(x) = \chi^\varepsilon(x)A + (1 - \chi^\varepsilon(x))B$$

where $\chi^\varepsilon(x)$ is the characteristic function of phase A . Obtaining estimates on A^* without being in position to explicitly compute A^* at a reasonable computational price is the whole interest of the approach by “bounds”.

3.1 The Hashin-Shtrikman bounds

Based on the density of the matrices obtained by periodic homogenization in the set of matrices obtained by arbitrary homogenization, it is possible to derive the following *Hashin-Shtrikman bounds* on A^* . In the sequel, we assume $B \geq A$.

Under the above assumptions, any homogenized matrix A^* satisfies the upper bound

$$A^*p \cdot p \leq Bp \cdot p + \theta \min_{\eta \in \mathbb{R}^d} [2p \cdot \eta + (B - A)^{-1}\eta \cdot \eta + (1 - \theta)h(\eta)] \quad (10)$$

for any $p \in \mathbb{R}^d$, where $h(\eta)$ is defined by

$$h(\eta) = \min_{k \in \mathbb{Z}^d, k \neq 0} \frac{|\eta \cdot k|^2}{Bk \cdot k}.$$

Similarly, any homogenized matrix A^* satisfies the lower bound

$$A^*p \cdot p \geq Ap \cdot p + (1 - \theta) \max_{\eta \in \mathbb{R}^d} [2p \cdot \eta - (B - A)^{-1}\eta \cdot \eta - \theta g(\eta)], \quad (11)$$

where $g(\eta)$ is defined by

$$g(\eta) = \max_{k \in \mathbb{Z}^d, k \neq 0} \frac{|\eta \cdot k|^2}{Ak \cdot k}.$$

Furthermore, the upper bound can always be attained: for any $p \in \mathbb{R}^d$, there exists a function χ , \mathbb{Z}^d -periodic and that generally depends on p , such that for the matrix A_p^* obtained by periodic homogenization of

$$A\left(\frac{x}{\varepsilon}\right) = \chi\left(\frac{x}{\varepsilon}\right)A + (1 - \chi\left(\frac{x}{\varepsilon}\right))B,$$

the inequality (10) becomes an equality (see *e.g.* [30]). Likewise, the lower bound (11) can always be attained. We have summarized in [1, Section 2.3.2] a proof of the Hashin Shtrikman bounds.

Remark 1 *Besides the Hashin-Shtrikman bounds, many other estimates have been proposed, such as the dilute approximation, the self-consistent method [31] and the Mori Tanaka methods [28]. They are all based on the fact that the problem of a single inclusion in an infinite material (Eshelby problem) is analytically solvable [23]. Similarly to the Hashin-Shtrikman bounds, the spatial distribution of the phases is not taken into account in these other bounds. The accuracy of these estimates and bounds strongly depends on the contrast between A and B and the volume fraction θ as shown on Figure 1 below.*

3.2 Numerical illustration

We consider a two-phase composite with A and B . We denote by a the scalar conductivity of A (respectively b the conductivity of B) with $a < b$. We denote by d the dimension, and by θ the volume fraction of A .

We consider the case of the random checkerboard, for which the exact homogenized matrix is known: $A^* = a^* \text{Id} = \sqrt{ab} \text{Id}$. In this simple case, the different bounds and estimates have an analytical form: the homogenized coefficient a^* is bounded from below by the harmonic mean (often called the Reuss bound) and from above by the arithmetic mean (often called the Voigt bound):

$$\frac{1}{\theta/a + (1 - \theta)/b} \leq a^* \leq \theta a + (1 - \theta)b.$$

These bounds are also called Wiener Bounds or Paul bounds. In this case, the Hashin-Shtrikman bounds detailed above read (see *e.g.* [25, page 188]):

$$a \left(1 + \frac{d(1-\theta)(b-a)}{da + \theta(b-a)} \right) \leq a^* \leq b \left(1 - \frac{d\theta(b-a)}{db + (1-\theta)(a-b)} \right),$$

and the Self-Consistent model leads to an estimate λ_{eff} of the effective conductivity a^* defined implicitly (see [26]) by

$$\theta \frac{a - \lambda_{\text{eff}}}{a + 2\lambda_{\text{eff}}} + (1 - \theta) \frac{b - \lambda_{\text{eff}}}{b + 2\lambda_{\text{eff}}} = 0.$$

On Figure 1 we plot these bounds and estimates for different values of the contrast, defined by b/a , for $a = 1$. Note that in this case, by construction, the volume fraction for any a and b is $\theta = 1/2$. In Tab. 1, we collect the values of all these bounds and estimates, for the particular case $a = 1$ and $b = 10$.

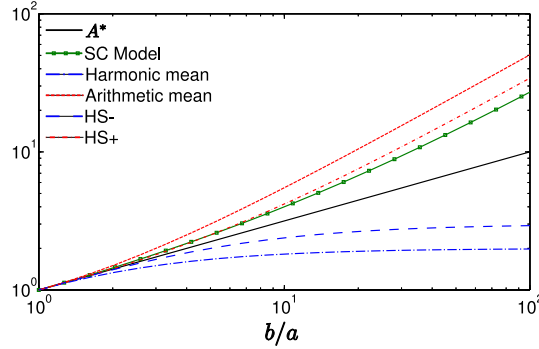


Figure 1: Different bounds for the checkerboard test case.

A^*	Harmonic	HS-	SC Model	HS+	Arithmetic
3.16	1.81	2.38	4.00	4.19	5.50

Table 1: Values of bounds and estimate for a contrast of $b/a = 10$.

We verify that, for the critical volume fraction $\theta = 0.5$, even for a contrast which is not extremely large ($a = 1$ and $b = 10$), the range of homogenized matrix atteignable, given by the Hashin-Shtrikman bounds, is *wide*. In such a case, the spatial distribution of phases, which is not taken into account on

the bounds, is certainly important. Note also that a typical case for real-world composites is more challenging than the case above, since the contrast is usually larger (of the order 100 rather than 10) and the volume fraction is similar.

Our numerical example therefore shows that, in many cases, *the Hashin Shtrikman bounds cannot provide accurate estimates of the homogenized matrix*. For a contrast of 10, the error between the bounds and A^* is larger than 25 %. For a contrast of 100, the upper bound is three times as large as the actual homogenized value, which is itself three times as large as the lower bound. *There is therefore a need for developing efficient numerical methods that provide more accurate results.*

4 A weakly-stochastic MsFEM approach

[Work expanded in [3].]

In this section, we show how the Multiscale Finite Element Method (MsFEM) can be adapted to the stochastic setting. We refer to [20] for a review on the MsFEM approach. Let us recall here that this method is designed to directly address the original problem (namely (5) in the case of interest here), keeping ε at its fixed value, rather than studying the limit problem when $\varepsilon \rightarrow 0$ (as we do in Section 2, going from (5) to (4)). Another interest of this method is that it does not require any explicit formula for the homogenized tensor (such as (2)-(3), or (6)-(7)), which are not always available. More details and comprehensive numerical tests are published in [3]. See also [4].

4.1 MsFEM approaches

For consistency and to set our notation, we briefly review the classical, deterministic setting for MsFEM approaches. We next turn to the stochastic setting. We consider problem (1), which we reproduce here for convenience,

$$\begin{cases} -\operatorname{div}(A^\varepsilon(x)\nabla u^\varepsilon(x)) &= f(x) \text{ in } \mathcal{D}, \\ u^\varepsilon &= 0 \text{ on } \partial\mathcal{D}, \end{cases} \quad (12)$$

where A^ε is a symmetric matrix satisfying the standard coercivity and boundedness conditions. Note that the approach is not restricted to the periodic setting, so we do not assume that $A^\varepsilon(x) = A(x/\varepsilon)$ for a periodic matrix A .

As recalled above, we wish here to keep ε fixed at a (small) given value. The MsFEM approach consists in performing a variational approximation of (12) where the basis functions are defined *numerically* and *encode the fast oscillations* present in (12). In the sequel we will argue on the variational formulation of (12):

$$\text{Find } u^\varepsilon \in H_0^1(\mathcal{D}) \text{ such that, } \forall v \in H_0^1(\mathcal{D}), \quad \mathcal{A}_\varepsilon(u^\varepsilon, v) = b(v), \quad (13)$$

where

$$\mathcal{A}_\varepsilon(u, v) = \sum_{i,j} \int_{\mathcal{D}} A_{ij}^\varepsilon(x) \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_j} dx \quad \text{and} \quad b(v) = \int_{\mathcal{D}} f v \, dx.$$

We introduce a classical P1 discretization of the domain \mathcal{D} , with L nodes, and denote ϕ_i^0 , $i = 1, \dots, L$, the basis functions.

Definition of the MsFEM basis functions Several definitions of the basis functions have been proposed in the literature (see *e.g.* [24, 21, 22, 14]). They give rise to different methods. In the following, we present one of these methods. We consider the problem

$$\begin{cases} -\text{div}(A^\varepsilon(x) \nabla \phi_i^{\varepsilon, \mathbf{K}}) = 0 & \text{in } \mathbf{K} \\ \phi_i^{\varepsilon, \mathbf{K}} = \phi_i^0|_{\mathbf{K}} & \text{on } \partial \mathbf{K}. \end{cases} \quad (14)$$

Note the similarity between (14) and the corrector problem (2). Note also that the problems (14), indexed by \mathbf{K} , are all independent from one another. They can hence be solved in parallel, using a discretization adapted to the small scale ε .

Macro scale problem We now introduce the finite dimensional space

$$\mathcal{W}_h := \text{span} \{ \phi_i^\varepsilon, \, i = 1, \dots, L \},$$

where ϕ_i^ε is such that $\phi_i^\varepsilon|_{\mathbf{K}} = \phi_i^{\varepsilon, \mathbf{K}}$ for all \mathbf{K} , and proceed with a standard Galerkin approximation of (13) using \mathcal{W}_h :

$$\text{Find } u_h^\varepsilon \in \mathcal{W}_h \text{ such that, } \forall v \in \mathcal{W}_h, \quad \mathcal{A}_\varepsilon(u_h^\varepsilon, v) = b(v). \quad (15)$$

The dimension of \mathcal{W}_h is equal to L : the formulation (15) hence requires solving a linear system with only a limited number of degrees of freedom.

Numerical illustration In order to illustrate the MsFEM approach, we solve (12) in a one dimensional setting with

$$A^\varepsilon(x) = 5 + 50 \sin^2 \left(\frac{\pi x}{\varepsilon} \right),$$

on the domain $\mathcal{D} = (0, 1)$, with $\varepsilon = 0.025$ and $f = 1000$. We subdivide the interval $(0, 1)$ in $L = 10$ elements. On Figure 2, we plot the MsFEM basis functions in a reference element and the MsFEM solution u_h^ε .

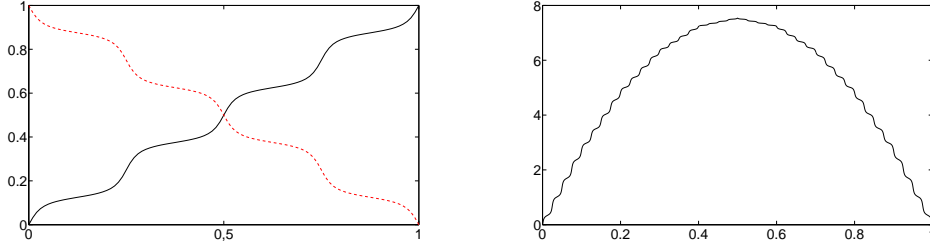


Figure 2: Left: Multiscale basis functions $\phi^{\varepsilon, \mathbf{K}}$ in the reference element. Right: MsFEM solution u_h^ε in the domain $(0, 1)$.

Natural adaptation to the stochastic setting When applied to the stochastic problem

$$\begin{cases} -\operatorname{div}(A^\varepsilon(x, \omega) \nabla u^\varepsilon(x, \omega)) &= f(x) \text{ in } \mathcal{D}, \\ u^\varepsilon &= 0 \text{ on } \partial\mathcal{D}, \end{cases} \quad (16)$$

where the practical issue is to build an estimate of the mean $\mathbb{E}(u^\varepsilon(x, \cdot))$ using a Monte-Carlo simulation method, the natural adaptation of the MsFEM method is the following: for each random realization m , first construct a MsFEM basis and next solve the macroscale problem. This approach requires a significantly large number of computations, since, for each realization, a new basis of oscillating functions is built, and a problem at the macroscale is solved. Such an approach has been described and analyzed in *e.g.* [18].

4.2 A weakly stochastic setting

As seen above, considering general random materials lead to extremely expensive computations. The question arises to know whether this general random context is really relevant, and whether adequate modifications can lead

to substantial improvements. Our line of thought here is based on the following two-fold observation: classical random homogenization is costly but perhaps, in a number of situations, not necessary. Many materials, albeit not deterministic, are not totally random. Some of them can be considered as a perturbation of a deterministic material. The homogenized behaviour should expectedly be close to that of the underlying deterministic material (and thus tractable from the practical viewpoint), up to an error depending on the amount of randomness present.

Model We introduce and study here a specific model for a randomly perturbed deterministic material (we refer to [12] for a quick overview of this setting, and some of the associated numerical techniques, and to [1] for a more comprehensive review of our contributions along these ideas). We are interested in the following elliptic problem

$$\begin{cases} -\operatorname{div} (A_\eta^\varepsilon(x, \omega) \nabla u_\eta^\varepsilon) &= f(x) & \text{in } \mathcal{D} \subset \mathbb{R}^d, \\ u_\eta^\varepsilon &= 0 & \text{on } \partial\mathcal{D}, \end{cases} \quad (17)$$

that is (16) with

$$A^\varepsilon(x, \omega) \equiv A_\eta^\varepsilon(x, \omega) = A_0^\varepsilon(x) + \eta A_1^\varepsilon(x, \omega), \quad (18)$$

where $\eta \in \mathbb{R}$ is a *small* parameter, A_0^ε is a deterministic matrix uniformly elliptic and bounded, and $A_1^\varepsilon(x, \omega)$ is a bounded matrix. The matrix A_η^ε is hence a *perturbation* of the deterministic matrix A_0^ε .

Remark 2 *The above setting is of course one possible setting where the theory may be developed. Other forms of random perturbations of deterministic (possibly periodic) problems could also be addressed. See e.g. [5, 6, 7, 8] and the review article [1].*

In the case (18), a MsFEM method alternative to the one presented in Section 4.1 can be proposed. The idea is to compute the MsFEM basis functions only *once*, with the *deterministic part* of the matrix A_η^ε and next to perform Monte-Carlo realizations only for the macro scale problems. We refer to [3] for all the details.

As above, we hence first solve (14), with $A^\varepsilon \equiv A_0^\varepsilon$, and build the finite dimensional space

$$\mathcal{W}_h := \operatorname{span} \{ \phi_i^\varepsilon, \ i = 1, \dots, L \}.$$

We next proceed with a standard Galerkin approximation of (17) using \mathcal{W}_h : for each $m \in \{1, \dots, M\}$, we consider a realization $A_\eta^{\varepsilon, m}(\cdot, \omega)$ and compute $u^m(\cdot, \omega) \in \mathcal{W}_h$ such that

$$\forall v \in \mathcal{W}_h, \quad \sum_{i,j} \int_{\mathcal{D}} (A_\eta^{\varepsilon, m})_{ij}(x, \omega) \frac{\partial u^m}{\partial x_i}(x, \omega) \frac{\partial v}{\partial x_j}(x) dx = \int_{\mathcal{D}} f(x) v(x) dx. \quad (19)$$

Since the MsFEM basis functions are only computed once, a large computational gain is expected, and this is indeed the case.

Numerical studies We now estimate the performance of the approach. To this aim, we compare the solution of the above approach with the solution of the direct approach (of Section 4.1) and, for reference, the solution to (17) obtained using a finite element method with a mesh size adapted to the small scale ε . Our estimators are built as follows:

$$e(u_1, u_2) = \mathbb{E} \left(\frac{\|u_1 - u_2\|_N}{\|u_2\|_N} \right), \quad (20)$$

where N is the norm used, u_1 and u_2 are the solutions obtained with any two different methods. The expectation is in turn computed using a Monte-Carlo method. Considering M realizations $\{X_m(\omega)\}_{1 \leq m \leq M}$ of a random variable (here $X(\omega) = \frac{\|u_1(\cdot, \omega) - u_2(\cdot, \omega)\|_N}{\|u_2(\cdot, \omega)\|_N}$), we compute the empirical mean μ_M and the empirical standard deviation σ_M as

$$\begin{aligned} \mu_M(X) &= \frac{1}{M} \sum_{m=1}^M X_m(\omega), \\ \sigma_M^2(X) &= \frac{1}{M-1} \sum_{m=1}^M (X_m(\omega) - \mu_M(X))^2. \end{aligned}$$

As a classical consequence of the Central Limit Theorem, it is commonly admitted that $\mathbb{E}(X)$ satisfies

$$|\mathbb{E}(X) - \mu_M(X)| \leq 1.96 \frac{\sigma_M(X)}{\sqrt{M}}.$$

We consider the following numerical example. Let $(X_{k,l})_{(k,l) \in \mathbb{Z}^2}$ denote a sequence of independent, identically distributed scalar random variables uniformly distributed over the interval $[0, 1]$. We define the random conductivity

matrix as

$$A_\eta^\varepsilon(x, y, \omega) = \sum_{(k,l) \in \mathbb{Z}^2} \mathbf{1}_{(k,k+1]}(\frac{x}{\varepsilon}) \mathbf{1}_{(l,l+1]}(\frac{y}{\varepsilon}) \left(\frac{2 + P \sin(2\pi x/\varepsilon)}{2 + P \sin(2\pi y/\varepsilon)} + \frac{2 + \sin(2\pi y/\varepsilon)}{2 + P \sin(2\pi x/\varepsilon)} \right) (1 + \eta X_{k,l}(\omega)) \text{Id}_2,$$

with the parameters $P = 1.8$ and $\varepsilon = 0.025$. Then we compute u_{ref} solution to (17) on the domain $\mathcal{D} = (0, 1)^2$, with $f \equiv 1$. Let u_M and u_S be its approximation by the general MsFEM approach (of Section 4.1) and the weakly-stochastic MsFEM approach described above, respectively. The numerical parameters for the computation are determined using an empirical study of convergence. We used for the reference solution a fine mesh of size $h_f = \varepsilon/40$. The MsFEM basis functions are computed in each element \mathbf{K} using a mesh of size $h_M = \varepsilon/80$. The coarse mesh size is $H = 1/30$. We consider $M = 30$ realizations.

We report in Tables 2 and 3 the estimator (20), along with its confidence interval, for the norms $H^1(\mathcal{D})$ and $L^2(\mathcal{D})$, respectively.

η	$e(u_M, u_{ref})$	$e(u_S, u_{ref})$	$e(u_S, u_M)$
1	8.12 ± 0.19	17.37 ± 0.78	15.51 ± 0.87
0.1	7.17 ± 0.02	7.62 ± 0.07	2.56 ± 0.10
0.01	7.15 ± 0.002	7.28 ± 0.007	1.39 ± 0.002

Table 2: $H^1(\mathcal{D})$ error (in %).

η	$e(u_M, u_{ref})$	$e(u_S, u_{ref})$	$e(u_S, u_M)$
1	0.56 ± 0.08	1.69 ± 0.49	1.47 ± 0.50
0.1	0.54 ± 0.01	0.57 ± 0.06	0.20 ± 0.07
0.01	0.53 ± 0.001	0.62 ± 0.005	0.11 ± 0.003

Table 3: $L^2(\mathcal{D})$ error (in %).

We observe that, when η is small (here, $\eta \leq 0.1$), the alternative approach provides a function u_S that is an approximation of u_{ref} as accurate as u_M . Recall that, since the MsFEM basis has only been computed once, the cost for obtaining an empirical approximation of $\mathbb{E}(u_S)$ is much smaller than that

for obtaining the corresponding empirical estimator of $\mathbb{E}(u_M)$. This demonstrates the efficiency of the approach. As expected, when η is not small (say $\eta \approx 1$), the accuracy of the solution u_S computed with the alternative approach proposed here decreases.

Elements of proof In [3], we have analyzed the method introduced here in the one-dimensional setting (see also [4]). For the sake of analysis, we assume that the highly oscillating coefficient reads $a_\eta^\varepsilon(x, \omega) = a_\eta\left(\frac{x}{\varepsilon}, \omega\right)$, where a_η satisfies the standard assumption of stochastic homogenization (see Section 2.2). The problem (17) now reads

$$\begin{cases} -\frac{d}{dx} \left(a_\eta\left(\frac{x}{\varepsilon}, \omega\right) \frac{d}{dx} u_\eta^\varepsilon(x, \omega) \right) = f(x) & \text{in } (0, 1), \\ u_\eta^\varepsilon(0, \omega) = u_\eta^\varepsilon(1, \omega) = 0. \end{cases} \quad (21)$$

We assume that the randomness is *small*, in the sense (see (18)) that

$$a_\eta(x, \omega) = a_{per}(x) + \eta a_1(x, \omega), \quad (22)$$

where a_{per} is a deterministic, periodic function and η is a *small* deterministic parameter.

In [3], we have bounded from above the difference between u_η^\star , the solution to the homogenized equation (4), and the weakly-stochastic MsFEM solution, in the following sense. For a given realization of the random coefficient $a_\eta(x, \omega)$, let $u(\cdot, \omega)$ be the weakly-stochastic MsFEM solution, that solves (19). By construction, this solution is a linear combination of the highly oscillating basis functions:

$$u(x, \omega) = \sum_{i=1}^L U_i(\omega) \phi_i^\varepsilon(x).$$

Let $v_{w-MsFEM}(x, \omega)$ be the associated representation in terms of standard P1 basis functions:

$$v_{w-MsFEM}(x, \omega) = \sum_{i=1}^L U_i(\omega) \phi_i^0(x).$$

We have the following estimate:

$$\|u_\eta^\star - v_{w-MsFEM}(\cdot, \omega)\|_{H^1(0,1)} \leq C \left(h + \frac{\varepsilon}{h} + \eta \sigma_h^\varepsilon(\omega) + \eta^2 \mathcal{C}(\eta) \right) \quad (23)$$

where C is a deterministic constant, independent of h , ε and η , and $\mathcal{C}(\eta)$ is a deterministic function, bounded when $\eta \rightarrow 0$. In the above bound, $\sigma_h^\varepsilon(\omega)$ is a random number, independent of η , that depends on ε , h and the random term $a_1(x, \omega)$ in (22).

Let us comment on (23). Assume that $\eta = 0$, i.e. the problem (21) is a periodic problem. Then our method is identical to the standard deterministic MsFEM method, and we recover from (23) the classical bound known in that case, namely

$$\|u_\eta^\star - v_{\text{MsFEM}}\|_{H^1(0,1)} \leq C \left(h + \frac{\varepsilon}{h} \right).$$

Assume now that a_1 is deterministic. Then our method is not exactly the MsFEM method, since we do not take into account a_1 to build the highly oscillating basis functions. In that case, $\sigma_h^\varepsilon(\omega)$ turns out to vanish, and we infer from (23) that

$$\|u_\eta^\star - v_{\text{w-MsFEM}}\|_{H^1(0,1)} \leq C \left(h + \frac{\varepsilon}{h} + \eta^2 \mathcal{C}(\eta) \right).$$

We hence observe that, provided the term neglected to build the basis functions is small (namely $\eta \ll 1$), we obtain a similar accuracy as with the standard MsFEM method.

A similar conclusion holds in the general case (22). Note also that the bound (23) is valid for any realization ω of the randomness. It is therefore a more precise result than a bound on the expectation of the error, where all random realizations are averaged. For instance, the bound (23) allows to understand what is the probability distribution of the error.

5 Conclusions and plan for the following years

In this report, we have first reviewed an approach to obtain bounds (here, the Hashin-Shtrikman bounds) on the homogenized matrix. This approach only involves computations of moderate difficulty. However, we have outlined the strong limitations of such a strategy. In some cases, the difference between the lower and upper bounds is indeed very large. The obtained estimations are then inaccurate. This motivates the development of efficient numerical methods that provide more accurate results.

To this aim, we have focused on weakly stochastic materials, for which we successfully adapted the well-known Multiscale Finite Element Method (MsFEM). We have proposed a method with a much smaller computational cost

than the original MsFEM in the stochastic setting. Provided the stochastic perturbation is indeed small, the method we propose is as accurate as the original one.

We summarize now the directions of research we wish to pursue during the following years.

A variant of classical random homogenization In the short term, our aim is to study a particular setting for stochastic homogenization, which is not the classical setting described in Section 2.2 (where the random coefficient A in (5) is stationary). The setting we wish to study is the case when the random coefficient is the composition of a standard deterministic and periodic function A_{per} with a stochastic diffeomorphism:

$$A^\varepsilon(x, \omega) = A_{\text{per}} \left[\Phi^{-1} \left(\frac{x}{\varepsilon}, \omega \right) \right] \quad (24)$$

where, for any random realization ω , the application $x \mapsto \Phi(x, \omega)$ is a diffeomorphism. Formally, such a setting models a microstructure that is periodic, in a given reference configuration. The latter is only known up to a certain randomness. Materials we have in mind are ideally periodic materials, where some random deformation has been introduced, for instance during the manufacturing process. Othewise stated, these are periodic materials seen through random glasses! This setting has been initially introduced in [9], where the homogenized problem is identified.

An interesting question in that context is that of numerical discretization. In the classical context, a standard procedure is to solve the corrector problem on a truncated domain (see (8) and (9)). The convergence of the procedure is given by [16, Theorem 1]. We currently work on a similar analysis in the context of (24) (see [2]).

A more theoretical question is to precisely understand the behaviour of $u^\varepsilon(x, \omega) - u^*(x)$ when ε goes to 0, where u^ε is the solution of the highly oscillating problem and u^* the solution of the homogenized problem. In the classical setting, and in the one-dimensional case, the convergence of $\varepsilon^{-1/2}(u^\varepsilon(x, \omega) - u^*(x))$ to a Gaussian process has been shown in [17]. This question, in the context of (24), is addressed in [2].

The setting (24) is in general not a weakly stochastic setting, as the amount of randomness present in Φ may be large. Yet, in the case when the diffeomorphism Φ is close to the identity, namely

$$\Phi(x, \omega) = x + \eta \Psi(x, \omega) + O(\eta^2) \quad (25)$$

for a small deterministic parameter η , the amount of randomness turns out to be small. This case is thus another instance of randomly perturbed deterministic materials (recall Section 4.2, where we introduced another weakly stochastic setting, and Remark 2, where we pointed out other weakly stochastic settings). The case (24)-(25) has been studied in [10, 11].

A Fast Fourier Transform approach In the course of our investigations, we have identified the following tracks of research, which are closely related to the research directions of the contract.

First, in the periodic homogenization setting recalled in Section 2.1, a method based on Fast Fourier Transform has been proposed in [29, 27]. The idea is as follows. Let A_0 be a constant symmetric positive matrix. The corrector problem (2) is equivalent to

$$\begin{cases} -\operatorname{div}(A_0(p + \nabla w_p)) = \operatorname{div}((A_{\text{per}}(y) - A_0)(p + \nabla w_p)) & \text{in } \mathbb{R}^d, \\ w_p \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases}$$

The idea of [29, 27] is to solve this problem iteratively. Knowing the iterate w_p^k at iteration k , the next iterate w_p^{k+1} is defined as the unique solution to

$$\begin{cases} -\operatorname{div}(A_0(p + \nabla w_p^{k+1})) = \operatorname{div}((A_{\text{per}}(y) - A_0)(p + \nabla w_p^k)) & \text{in } \mathbb{R}^d, \\ w_p^{k+1} \text{ is } \mathbb{Z}^d\text{-periodic.} \end{cases}$$

As A_0 is a tensor independent of y (in contrast to $A_{\text{per}}(y)$), the above problem can be solved very efficiently using a Fourier transform. Hence, rather than solving (2), we are left with solving many times a simpler problem.

Our aim is to compare this iterative method with the standard method, in term of efficiency. The choice of A_0 is most probably of paramount importance, since the convergence rate (and also the fact that the iterations in k converge or not) depends on it. We have already run some preliminary tests with this method, but definite conclusions are yet to be obtained.

Second, in the context of stochastic homogenization, approaches using some decomposition of the random matrix $A(x, \omega)$ in (5) would be worthwhile to investigate.

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